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VAPOR-PHASE INFRARED ABSORPTIVITY COEFFICIENT OF CYCLOHEXYL ISOTHIOCYANATE

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| 14. ABSTRACT We measured the vapor-phase absorptivity coefficient of cyclohexyl isothiocyanate in the mid-infrared (4000-550 cm ⁻¹) at a spectral resolution of 0.125 cm ⁻¹ . The chemical used in the feedstock was subjected to a rigorous analysis by gas chromatography-mass spectrometry, nuclear magnetic resonance, and Karl-Fischer titration to verify its purity. We describe the experimental method used to acquire the individual spectra that were used to produce the composite spectrum and summarize the statistical uncertainties in the data. | | | | | | | | | | | | | | | |
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EXECUTIVE SUMMARY

We measured the vapor-phase absorptivity coefficient of cyclohexyl isothiocyanate (CHNCS) at a spectral resolution of 0.125 cm^{-1} . We used saturator cells suspended in a temperature controlled liquid bath to generate continuous streams of CHNCS diluted in nitrogen. The vapor was then sent to a variable path White cell and measured using a high resolution research grade Fourier Transform Infrared Spectrometer. The purity of the feedstock was verified by gas chromatography, nuclear magnetic resonance, and Karl-Fischer titration. The concentration of CHNCS in the vapor was determined with a gravimetric method. Eleven spectra at different concentration path-length products were processed line by line through least squares analysis using MatLab® to produce the absorptivity coefficient of the compound and the statistical uncertainty in the data. Uncertainties in the data, expanded to a confidence interval of 2σ ($P=0.95$) are Type-A: 1.2% and Type-B: 3.9% of the absorptivity coefficient. To our knowledge, the vapor-phase absorptivity coefficient of this compound has not been published previously.

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PREFACE

The work described in this report was performed under the direction of the Detection Capability Officer, Defense Threat Reduction Agency Joint Science and Technology Office. This work was started and completed in April 2008.

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VAPOR-PHASE INFRARED ABSORPTIVITY COEFFICIENT OF CYCLOHEXYL ISOTHIOCYANATE

1. INTRODUCTION

We have obtained the high resolution vapor-phase absorptivity coefficients of cyclohexyl isothiocyanate (CHNCS) in the spectral range of 4000-550 cm^{-1} in units of $(\mu\text{mol/mol})^{-1}\text{m}^{-1}$. We also report the uncertainties of the data.

Cyclohexyl isothiocyanate has the Chemical Abstracts Service (CAS) Registry Number 1122-82-3 and is indexed under cyclohexane, isothiocyanato. The molecular formula of CHNCS is $\text{C}_7\text{H}_{11}\text{NS}$, and it has a molecular weight of 141.24. The structure is shown in Figure 1.

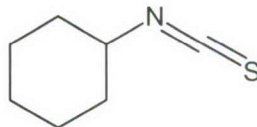


Figure 1. Structure of Cyclohexyl Isothiocyanate

Cyclohexyl isothiocyanate is a liquid at room temperature, with a boiling point of 219 °C (96-98 °C at 10-Torr). At the time of study, we were unable to find vapor pressure data for the compound in the ambient temperature range. Cyclohexyl isothiocyanate is frequently observed in samples of VX nerve agent because one of the stabilizers frequently used in nerve agent formulations, dicyclohexyl carbodiimide, can chemically react with VX or its degradants to produce the isothiocyanate compound. The CHNCS would be expected to have a significantly greater volatility than VX. Non-quantitative vapor-phase Fourier transform infrared (FTIR) spectra of the compound have indicated in the past that several absorption features in the fingerprint region gave it the potential to be an interferent for standoff detection of VX.

2. EXPERIMENTAL PROCEDURES

2.1 Instrumental Details

The system used to generate the continuous vapor stream was an adaptation of the saturator cell method developed at the U.S. Army Edgewood Chemical and Biological Center (ECBC) for measuring the volatility of chemical warfare (CW) agent related compounds.¹

The method, modified to generate continuous streams of chemical compounds for obtaining quantitative vapor-phase IR spectra, has been used to measure the absorptivity coefficients of benzene², as well as a variety of CW agent related compounds.³ The saturator passes a stream of nitrogen carrier gas, obtained from the boiloff of a bulk liquid nitrogen tank, across a conical alumina wicking mechanism in a glass holder filled with the analyte. A saturated vapor-liquid equilibrium of the analyte on the downstream side of the saturator cell

results with the concentration of the analyte determined by the temperature of the liquid phase. By suspending the saturator cell in a constant temperature bath, the concentration of the analyte can be predicted by its vapor pressure at the temperature of the bath. The apparatus used in the Quantitative Fourier transform infrared spectrometer (FTIR) Laboratory used a Brooks Model 5850S (Emerson, Hatfield, PA) mass flow controller to maintain a constant flow to the saturator cell. A second mass flow controller was used to add diluent to the stream, providing an additional means of adjusting the concentration of the compound delivered to the White cell of the FTIR. Linearity of the S series mass flow controllers is adjusted using a second order polynomial, resulting in accuracies of approximately 1% or better of rate at flows $\geq 25\%$ of full scale.

Spectra were obtained with a Bruker Model IFS/66V FTIR. The instrument is equipped with deuterated triglycine sulfide and mercury-cadmium-telluride (HgCdTe) detectors and is capable of obtaining spectra with a maximum spectral resolution of 0.1125 cm^{-1} (unapodized). The interferograms were recorded from $15798\text{--}0\text{ cm}^{-1}$ with a resolution of 0.125 cm^{-1} . Absorbance (log base-10) spectra were processed with boxcar apodization and 2X zero filled to obtain a data spacing of 0.0625 cm^{-1} . The instrument is equipped with a variable path White cell. The experimental data used path lengths of 1.405, 2.727, 4.057, 5.377, and 8.024 m. The temperature of the White cell was maintained at $23 \pm 0.1\text{ }^{\circ}\text{C}$ through the use of a thermostatically controlled chamber enclosing the spectrometer and cell. Data were acquired at a speed of 60 KHz (HeNe laser zero crossing frequency) using the HgCdTe detector. Absorbance spectra of the compound were computed using background spectra of clean, dry nitrogen. To minimize the effects of nonlinearity in the detector, the interferograms were processed using the proprietary Opus® nonlinearity correction function. All interferograms have been archived enabling further post-processing of data.

Temperature and pressure data were recorded using NIST traceable digital manometers and thermometers, and all data have been archived. Concentration path-length products (CL) were computed in units of $\mu\text{mol/mol(m)}$ (ppm-m). A differential pressure manometer had previously been used to measure the dynamic pressure in the White cell with gas flowing into the cell. The ambient pressure was plotted versus the differential pressure. The resulting equation was used to correct the readings from the ambient pressure manometer to the pressure in the White cell. The concentration-path-length data were corrected to 296 K and $1.0132 \times 10^5\text{ Pa}$ (760 Torr), using the ideal gas law.

2.2 Feedstock

The material used to generate the vapor streams for the experiments was obtained from Sigma-Aldrich (Milwaukee, WI) (cat. no. C105406-25G, lot no. 02929CO), with a reported purity of 98%.

Aliquots of the compound were analyzed by the following three independent methods: GC-mass spectrometry, GC-FTIR, and NMR. The GC-MS returned a purity of 99.76 area%. The more volatile impurity (based upon its GC retention time) was present at 0.076 area%, with a mass spectrum showing the presence of at least two chlorine atoms in the molecule. Although a library search returned a match with 1,2-dichloro-1-fluoroethylene,

the spectrum of the impurity had an ion at m/z 76, not seen in the library spectrum. Because such an ion would be difficult to explain mechanistically, it is likely that the peak in the chromatogram either comprised two co-eluting compounds, or we were seeing the fragments of a different compound with a mass spectrum similar to that of the library match. We compared the vapor-phase spectra of the effluent from the saturator cell obtained during the first day's run with those obtained during the remaining trials and analyzed the statistical uncertainties in the least squares fit of the absorptivity coefficient. These indicated that the impurity might have absorption bands centered at 1535 cm^{-1} (P-R), 1270 cm^{-1} (P-Q-R), and 760 cm^{-1} (possible P-Q-R). The frequencies of the IR bands and apparent rotational fine structure would be consistent with a simple unsaturated halogenated compound (e.g., a haloalkene). Analysis of the residuals indicated that the impurities contributed $<1\%$ of the integrated area of the spectra obtained on the first day. Their contribution decreased on subsequent days as the impurities were purged from the feedstock.

The less volatile of the two impurities observed by GC-MS was present at 0.16 area% and had a mass spectrum indicating the presence of at least three chlorine atoms in the molecule, with a fragmentation pattern similar to that of the earlier eluting impurity. It yielded only a poor library match.

The NMR (proton) analysis yielded a purity of 99.73%. The concentration of the impurity that was observed was too small to obtain a definitive structure.

A Karl-Fischer titration of the feedstock compound was performed, giving a concentration of water at 30 parts-per-million (ppm). Trace water vapor was observed in the IR spectra of the effluent obtained during the first day's run, and the features were removed from the spectra by spectral subtraction.

3. RESULTS AND DISCUSSION

Four trials were run to obtain spectra at eleven concentration path-length products. A trial is defined as filling and weighing the saturator cell; suspending it in the bath; applying a stream of nitrogen for a measured time; acquiring several spectra; stopping the nitrogen and removing it from the bath; and reweighing the saturator cell after drying the exterior surfaces and re-equilibrating to room temperature. The trials were conducted at a bath temperature of $24.0\text{ }^{\circ}\text{C}$.

A fifth experiment, also at $24.0\text{ }^{\circ}\text{C}$, was run to obtain a vapor pressure for the compound in the ambient temperature range. The theoretical basis for the method is that the vapor generation system used produces a saturated vapor-liquid equilibrium, with the mass rate proportional to the vapor pressure. The procedure and calculations for obtaining vapor pressure from saturator cell data are explained in more detail in a previously published report.¹ A carrier flow rate of 100 standard cubic centimeters per minute (sccm) was maintained for 28 hr, resulting in a delta mass of 0.1490 g, yielding a vapor pressure of 0.115 ± 0.002 Torr (15.3 Pa). Because of the paucity of vapor pressure data for this compound, we used the ambient temperature vapor pressure datum from our experiment, along with the two other points,

760 Torr at 219 °C (B.P.) and 10 Torr at 97 °C (from the manufacturer), to fit the Antoine vapor pressure coefficients. The mathematical concept has been described by Penski, who used a basic program to compute the coefficients of a number of CW-related compounds.⁴ We use MatLab to run the computations, which uses a least squares fit to calculate a, b, and c for the linear equation seen in Figure 2. Using the coefficients in Figure 2 yields a vapor pressure of 0.124 Torr at 25 °C. We acknowledge that using only three data points across such a wide range certainly limits the accuracy of the resulting calculations of the vapor pressure of the compound for any temperature between the known points. We would note that, although low, its vapor pressure is apparently still nearly 150 times greater than that of VX (0.00079 Torr at 24 °C, using Antoine coefficients from Buchanan, et al.⁵). We believe, therefore, that the data provide a useful starting point for estimating the contribution of CHNCS to the ambient temperature spectrum of VX.

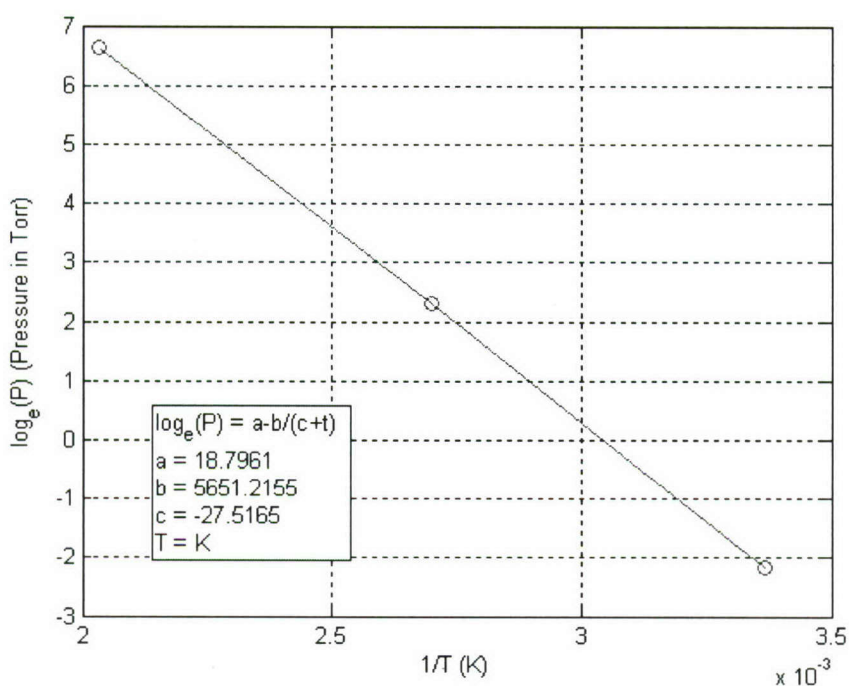


Figure 2. Vapor Pressure of Cyclohexyl Isothiocyanate and Antoine Coefficients

Before computing the absorptivity coefficient of the CHNCS, baseline corrections of the raw spectra were performed using a two point linear subtraction using an algorithm written in MatLab. The correction in all cases was $<0.0015 A$ [$A = -\log_{10}(T)$].

The composite spectrum (absorptivity coefficient) was computed using spectra with concentration-path-length products ranging 37-443 $\mu\text{mol/mol(m)}$ (corrected to 296 K and 101325 Pa). As an initial check of the quality of the data, Beer's Law plots of two spectral lines, 2946 and 2059 cm^{-1} , were calculated using MatLab. For at least these two spectral lines, the data appeared to be well fitted. There were no points lying outside of the 95% confidence limits for either a repeated set, a repeated single x, or the 95% confidence limits for a Grubbs Test for Outliers (Figures 3 and 4).

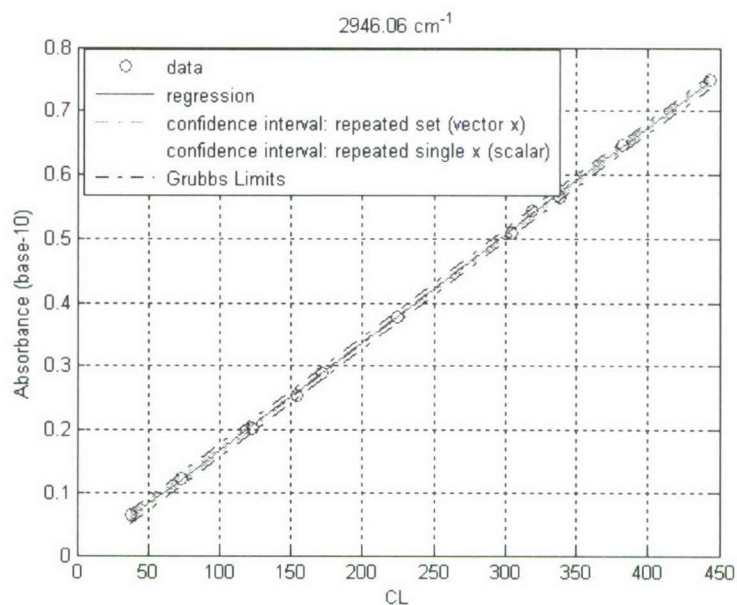


Figure 3. Beer's Law Plot of 2946 cm^{-1} Line in the Vapor-Phase Spectrum of Cyclohexyl Isothiocyanate

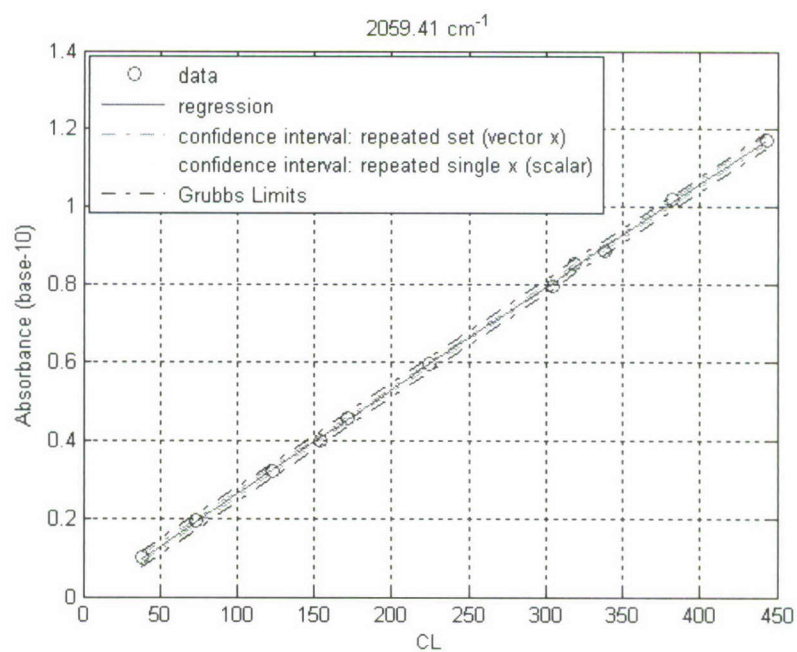


Figure 4. Beer's Law Plot of 2059 cm^{-1} Line in the Vapor-Phase Spectrum of Cyclohexyl Isothiocyanate

The absorptivity coefficient (α) and uncertainty (Type-A, 2σ) were computed line by line within the spectral range of 4000-550 cm^{-1} using a MatLab program written in-house. Values of ($A=-\log T$) >1.5 are normally assigned a weight of zero. Because A in all cases was <1.2 , all values of A were weighted at 1. Figure 5 is the plotted absorptivity coefficient (α) and uncertainty (U_α). The figure is plotted with α in $(\mu\text{mol}/\text{mol})^{-1}\text{m}^{-1}$. To obtain α in $(\text{mg}/\text{m}^2)^{-1}$, multiply the values in the mantissa of Figure 3 by 0.1710. This factor is derived from eq 1 using the molecular weight of CHNCS (141.24).

$$\frac{m^2}{\text{mg}} \left(\frac{24.15}{mw} \right) = \frac{\text{mol}}{\mu\text{mol}(m)} \quad (1)$$

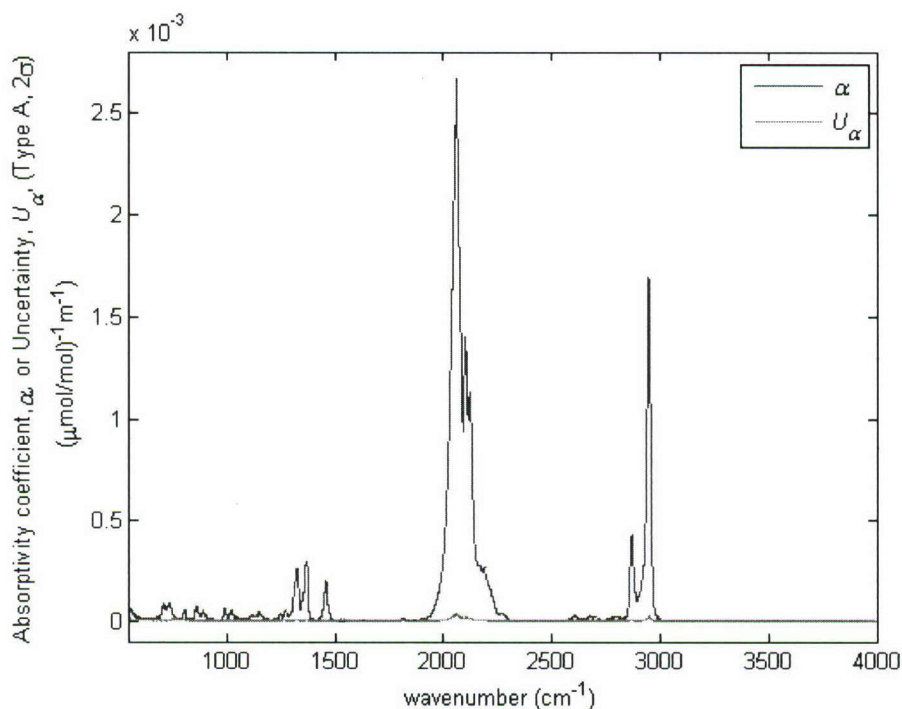


Figure 5. Absorptivity Coefficient and Type-A Uncertainty (2σ) of Cyclohexyl Isothiocyanate

Table 1 provides the absorptivity coefficients in $(\mu\text{mol}/\text{mol})^{-1}\text{m}^{-1}$ and $(\text{mg}/\text{m}^2)^{-1}$ for selected bands in units of wave number and micrometers.

Table 1. Absorptivity Coefficient of Cyclohexyl Isothiocyanate for Selected Bands

| Wavenumber, cm^{-1} (Wavelength, μm) | Absorptivity coefficient, $(\mu\text{mol}/\text{mol})^{-1}\text{m}^{-1}$ [(mg/m^2) $^{-1}$] |
|--|---|
| 2446.06 (3.394) | 1.692E-03 (2.893E-04) |
| 2059.26 (4.856) | 2.659E-03 (4.547E-04) |
| 1363.98 (7.331) | 2.975E-04 (5.088E-05) |
| 989.01 (10.111) | 6.328E-05 (1.082E-05) |

In general, expanded type-A uncertainties were 1-1.5% of the absorptivity coefficient, as seen in Figure 6 and 7. Figure 6 is a plot of absorptivity coefficients (abscissa) and fractional uncertainty (Type-A, U_A , 2σ) (mantissa). Figure 7 is a plot of the absorptivity coefficient and uncertainty and also includes a best fit of the data points obtained by least squares, which is an approximation of $U_A \approx ax+b$. For the fitted line in Figure 8, the coefficients are $a = 1.24 \times 10^{-2}$ and $b = 1.95 \times 10^{-6}$ (Table 2).

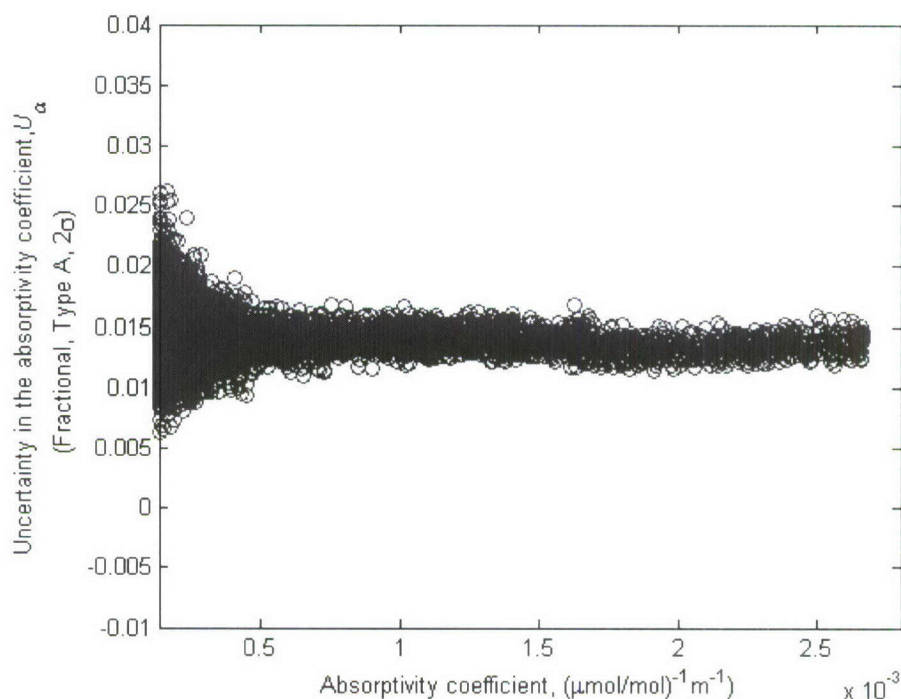


Figure 6. Absorption Coefficient (Abscissa) and Type-A Uncertainty (2σ) for Cyclohexyl Isothiocyanate

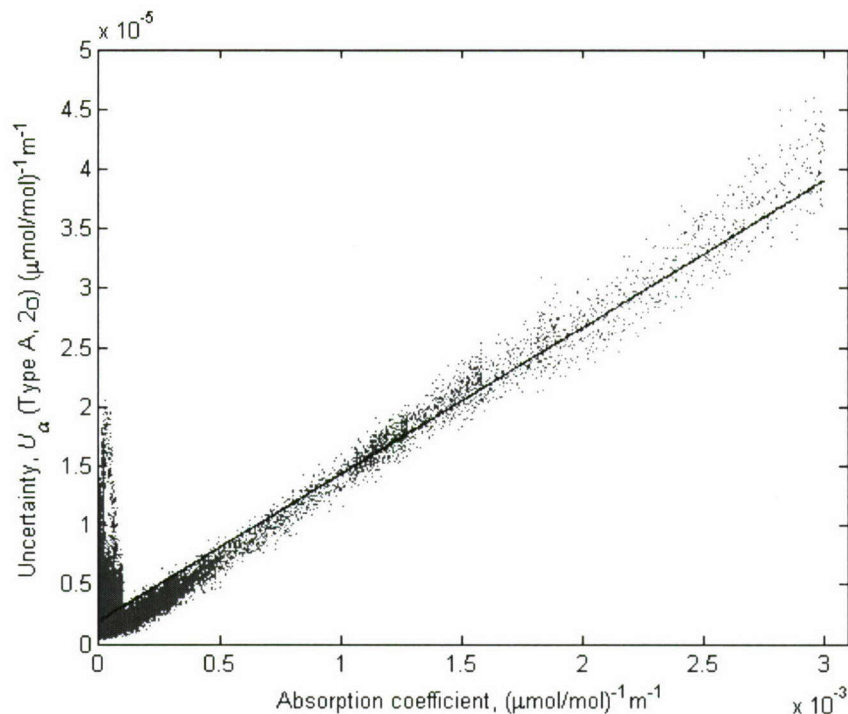


Figure 7. Absorption Coefficient (abscissa) and Type-A Fractional Uncertainty (2σ) for Cyclohexyl Isothiocyanate

Table 2. Type-A Statistical Uncertainty for Cyclohexyl Isothiocyanate Vapor-Phase Absorptivity Coefficient

| Type A $2\sigma \approx ma + b$ | |
|------------------------------------|-----------------------|
| Slope m | Intercept b |
| 1.24×10^{-2} | 1.95×10^{-6} |

Type-B estimated standard errors, along with their sources, as well as the combined Type-A and B uncertainties are provided in Table 3. The expanded combined Type-B uncertainty was computed using eq 2.

$$\Delta_B = (\Delta L^2 + \Delta T^2 + \Delta P^2 + \Delta \text{FTIR}^2 + \Delta \text{NL}^2 + \Delta \text{MR}^2)^{1/2} \quad (2)$$

The sources of uncertainty and their fractional values, as well as an explanation of the symbols in eq 1 are given in Table 4. Among the Type-B uncertainties, the purity dominates at 0.0075 (1σ).

Table 3. Uncertainties in Absorptivity Coefficient of Cyclohexyl Isothiocyanate from ECBC Data where $\alpha \geq 0.000133 \text{ (}\mu\text{mol/mol)}^{-1} \text{ m}^{-1}$

| Symbol | Fractional Deviation | Source |
|------------------------|----------------------|--------------------------------|
| ΔL | 0.005 | Pathlength |
| ΔT | 0.0006 | Temperature of White cell |
| ΔP | 0.0003 | Pressure |
| ΔFTIR | 0.0005 | Drift in spectrometer |
| ΔNL | 0.01 | Nonlinearity in detector |
| ΔMR | 0.005 | Mass rate |
| ΔD | 0.005 | Dilution rate |
| Δpurity | 0.0075 | Purity of feedstock |
| Δ_B | 0.03 | Combined type B (2σ) |
| Δ_A | 0.027 | Type-A deviation (2σ) |

We were unable to find another source of high-resolution quantitative vapor-phase IR spectra of this compound for comparison.

4. CONCLUSIONS

The vapor-phase absorptivity coefficient of cyclohexyl isothiocyanate was measured within the range $4000\text{-}550 \text{ cm}^{-1}$. Combined uncertainties, expanded to 2σ , are Type-A: 2.7% and Type-B: 3% of the absorptivity coefficient at intensities $\geq 5\%$ of the most intense absorption feature.

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